5 Numerical solution of the radial Schrödinger equation

In the last lecture we computed analytically phase shifts for several trivial examples of short-range interaction potentials. However, in most realistic situations an analytic solution is not available. Therefore we have to use numerical techniques to solve the radial equation

$$\left[\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k^2 - U(r) \right] u_l(kr) = 0, \tag{5.1}$$

$$U(r) = 2m/\hbar^2 V(r), \tag{5.2}$$

with the boundary condition at origin

$$u_l(0) = 0. \tag{5.3}$$

We are assuming that the potential $U(r)$ is short-range, i.e. it satisfies the conditions (4.15). This allows us to preform the matching at a finite radius, $r > r_0$, where $U(r) << \frac{l(l+1)}{r^2}$ and the particle can be considered free. For scattering calculations we only need the phase shift $\delta_l(k)$ which can be used to compute all observables. This quantity is obtained by matching the numerically determined solution $u_l(kr)$ to the free form valid for $r > r_0$

$$u_l(kr) = N[\cos(\delta_l(k))\hat{j}_l(kr) + \sin(\delta_l(k))\hat{n}_l(kr)]. \tag{5.4}$$

Asymptotically, this solution behaves as

$$u_l(kr) \sim \sin(kr - l\pi/2 + \delta_l(k)), r \to \infty. \tag{5.5}$$

5.1 Numerov method

This is a simple, yet for our purposes a sufficiently efficient method for computation of scattering and bound solutions of (5.1). In fact the method can be used to solve even inhomogeneous forms of (5.1) and applied to solve e.g. Poisson equation or to find the regular solution, see Chapter 8. We will derive the working equations of the method for the inhomogeneous case and then specialize it for solution of (5.1). We start by rewriting the equation using a simplified notation:

$$\frac{d^2}{dr^2}\Psi(r) + k^2(r)\Psi(r) = S(r), \tag{5.6}$$

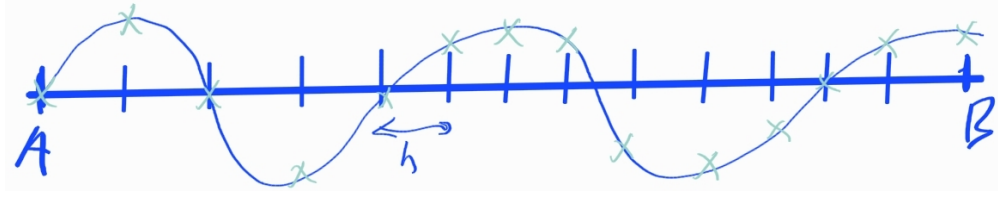$$k^2(r) = k^2 - \frac{l(l+1)}{r^2} - U(r). \tag{5.7}$$

Figure 5.1: In the Numerov method the selected interval $[A, B]$ is discretized with a constant step of size h. The wavefunction is then represented as a set of numbers representing its values in this interval.

Here $k(r)$ can be thought of as the instantaneous momentum of the particle and $S(r)$ is the source term.

To solve this equation numerically requires requires replacing the derivative $\frac{d^2}{dr^2}\Psi(r)$ with a suitable approximation. We start by discretizing space with equal step h, see Fig. 5.1. Thus the function $\Psi(r)$ becomes a set of values $\Psi_i = \Psi(r_i)$, $i = 1, \ldots, n$, representing the values of the function on the grid. Derivative of a function can be approximated with the help of Taylor expansion

$$\Psi_{n+1} = \Psi_n +$$
$$h\Psi'_n + \frac{h^2}{2}\Psi''_n + \frac{h^3}{3!}\Psi'''_n + \frac{h^4}{4!}\Psi''''_n + \frac{h^5}{5!}\Psi^v_n + O(h^6), \quad (5.8)$$
$$\Psi_{n-1} = \Psi_{n-1} -$$
$$h\Psi'_{n-1} + \frac{h^2}{2}\Psi''_{n-1} - \frac{h^3}{3!}\Psi'''_{n-1} + \frac{h^4}{4!}\Psi''''_{n-1} - \frac{h^5}{5!}\Psi^v_{n-1} + O(h^6). \quad (5.9)$$

The contributions of odd powers of h are eliminated by taking the following linear combination of the preceding two equations

$$\Psi_{n+1} - 2\Psi_n + \Psi_{n-1} = h^2\Psi''_n + \frac{h^4}{12}\Psi''''_n + O(h^6). \quad (5.10)$$

The last equation is probably a familiar expression for you. If we neglected the term proportional to Ψ''''_n we could approximate the second derivative of a function to order $O(h^2)$:

$$\frac{\Psi_{n+1} - 2\Psi_n + \Psi_{n-1}}{h^2} = \Psi''_n + O(h^2). \quad (5.11)$$

However, we can do much better utilizing Eq (5.6) to approximate also the fourth derivative in Eq (5.10):

$$\Psi''''_n = \frac{d^2}{dr^2}\left[S(r) - k^2(r)\Psi(r)\right]\bigg|_{r=r_n} = \frac{d^2}{dr^2}\left[t(r)\right]\bigg|_{r=r_n}, \quad (5.12)$$

where we have defined $t(r) = S(r) - k^2(r)\Psi(r)$. We can now approximate the last expression and obtain

$$\frac{d^2}{dr^2}\left[t(r)\right]\bigg|_{r=r_n} = \frac{1}{h^2}\left[t_{n+1} - 2t_n + t_{n-1}\right] + O(h^2). \quad (5.13)$$

Note that we've not written out the higher order term proportional to t_n'''' since we don't need it: when Eq (5.13) is inserted into Eq (5.10) we find that to order $O(h^6)$ we have

$$\Psi_{n+1} - 2\Psi_n + \Psi_{n-1} = h^2\Psi_n'' + \frac{h^2}{12}\left[t_{n+1} - 2t_n + t_{n-1}\right] + O(h^6), \tag{5.14}$$

since $h^4 O(h^2) = O(h^6)$. Clearly, this is two orders of magnitude better approximation than the one we would have had obtained in the lowest order approximation Eq (5.11). Therefore our approximation for the second derivative from Eq (5.6) is

$$\frac{d^2}{dr^2}\Psi(r)\bigg|_{r=r_n} = \frac{1}{h^2}\left[\Psi_{n+1} - 2\Psi_n + \Psi_{n-1}\right] - \frac{1}{12}\left[t_{n+1} - 2t_n + t_{n-1}\right] + O(h^4). \tag{5.15}$$

We now insert this result back into Eq (5.6), substitute for $t(r) = S(r) - k^2(r)\Psi(r)$ and simplify with the goal to isolate the terms multiplying Ψ_{n+1}, Ψ_n and Ψ_{n-1}:

$$\frac{1}{h^2}\left[\Psi_{n+1} - 2\Psi_n + \Psi_{n-1}\right] - \frac{1}{12}\left[t_{n+1} - 2t_n + t_{n-1}\right] = t_n, \tag{5.16}$$

$$\frac{1}{h^2}\left[\Psi_{n+1} - 2\Psi_n + \Psi_{n-1}\right] - \frac{1}{12}\left[t_{n+1} + 10t_n + t_{n-1}\right] = 0, \tag{5.17}$$

$$\frac{1}{h^2}\left[\Psi_{n+1} - 2\Psi_n + \Psi_{n-1}\right] -$$
$$\frac{1}{12}\left[S_{n+1} - k_{n+1}^2\Psi_{n+1} + 10S_n - 10k_n^2\Psi_n + S_{n-1} - k_{n-1}^2\Psi_{n-1}\right] = 0, \tag{5.18}$$

$$\Psi_{n+1}(1 + \frac{h^2}{12}k_{n+1}^2) - 2\Psi_n(1 - \frac{5h^2}{12}k_n^2) + \Psi_{n-1}(1 + \frac{h^2}{12}k_{n-1}^2) -$$
$$\frac{h^2}{12}(S_{n+1} + 10S_n + S_{n-1}) = 0. \tag{5.19}$$

The last equation could be used to solve the inhomogeneous Schrödinger equation. However, here we specialize to the homogeneous case and finally obtain

$$\Psi_{n+1}(1 + \frac{h^2}{12}k_{n+1}^2) - 2\Psi_n(1 - \frac{5h^2}{12}k_n^2) + \Psi_{n-1}(1 + \frac{h^2}{12}k_{n-1}^2) = 0. \tag{5.20}$$

Application of the method is straightforward. To propagate towards larger r express Ψ_{n+1} in terms of the function values at the two previous points Ψ_n and Ψ_{n-1}. To propagate towards smaller r express Ψ_{n-1} in terms of Ψ_n and Ψ_{n+1}. This way the solution can be obtained given two neighbouring values of the wavefunction.

How do we obtain the starting values? For scattering problems we make use of the boundary condition at $r = 0$ and set

$$\Psi_0 = 0, \tag{5.21}$$
$$\Psi_1 = A, \tag{5.22}$$

where A is an arbitrary constant. It is OK to leave the constant A arbitrary because we have not fixed normalization of the wavefunction: the Schrödinger equation is linear so a solution multiplied by an arbitrary constant also solves the equation. For bound solutions the principle is similar and will be explained below.

5.1.1 Phase shifts

In scattering problems energy is fixed and the task is to find the phase shift. To do that we need to use Eq (5.20) to propagate from $r = 0$ all the way to the potential-free region $r > r_0$. Let r_1 and $r_2 > r_1$ be two points (not necessarily close) in this region, see Fig. 5.2a. Then the solution at those two points is given by Eq (5.4)

$$\Psi(r_1) = N[\cos(\delta_l(k))\hat{j}_l(kr_1) + \sin(\delta_l(k))\hat{n}_l(kr_1)], \qquad (5.23)$$

$$\Psi(r_2) = N[\cos(\delta_l(k))\hat{j}_l(kr_2) + \sin(\delta_l(k))\hat{n}_l(kr_2)], \qquad (5.24)$$

where N is an arbitrary normalization of the wavefunction. We want to match our numerical solution (the left hand sides) to this form. The two equations above constitute a set of two equations for two unknowns. However, since we only need the phase shift we take the ratio of the two equations to dispense with the normalization

$$\frac{\Psi(r_1)}{\Psi(r_2)} = G = \frac{\cos(\delta_l(k))\hat{j}_l(kr_1) + \sin(\delta_l(k))\hat{n}_l(kr_1)}{\cos(\delta_l(k))\hat{j}_l(kr_2) + \sin(\delta_l(k))\hat{n}_l(kr_2)}. \qquad (5.25)$$

Eliminating the $\cos(\delta_l(k))$ term we obtain after trivial manipulations

$$\tan\delta_l(k) = \frac{\hat{j}_l(kr_1) - G\hat{j}_l(kr_2)}{G\hat{n}_l(kr_2) - \hat{n}_l(kr_1)}, \qquad (5.26)$$

where G is the value obtained from numerical intergation. From this equation the phase shift can be calculated to within an arbitrary multiple of π.

5.1.2 Bound states

When we search for bound states the task is reversed: the boundary conditions are fixed and we look for the eigenenergy E. One method of obtaining bound states is the shooting method which propagates from $r = 0$ and looks for energies which result in wavefunctions decaying to zero at $r >> r_0$. This way all eigenenergies can be in principle determined. However, it turns out that this approach may become numerically unstable on account of admixture of an exponentially increasing solution (this is the second independent and unphysical, solution of the radial Schrödinger equation in the classically forbidden region), see below. A numerically stable approach is obtained propagating from **both** sides: from zero and from a large (asymptotic) radius. Energy of the bound state is then found by **smoothly** matching the two solutions at some fixed matching radius r_M, see Fig. 5.2b.

To perform the matching we first need to normalize one strand of the solution so that $\Psi_<(r_M) = \Psi_>(r_M)$. Then we are ready to test matching of the derivatives. Let $\frac{d\Psi_<}{dr}$ and $\frac{d\Psi_>}{dr}$ be the derivatives of the propagated wavefunction at $r = r_M$ obtained by propagating inwards and outwards, respectively

$$\frac{d\Psi_<}{dr} \approx \frac{\Psi_<(r_M) - \Psi_<(r_{M-1})}{h}, \qquad (5.27)$$

$$\frac{d\Psi_>}{dr} \approx \frac{\Psi_>(r_M) - \Psi_>(r_{M-1})}{h}. \qquad (5.28)$$

Then the condition for their equality is written as:

$$\frac{d\Psi_<}{dr} - \frac{d\Psi_>}{dr} \approx \frac{\Psi_<(r_M) - \Psi_<(r_{M-1}) - \Psi_>(r_M) + \Psi_>(r_{M-1})}{h} = \quad (5.29)$$

$$\frac{\Psi_>(r_{M-1}) - \Psi_<(r_{M-1})}{h} = 0. \quad (5.30)$$

A reasonable choice for the position of the matching point is close to the point where the wavefunction has it is first local maximum, i.e. $\Psi_>(r_{n+1})/\Psi_>(r_n)$, see Fig. 5.2b.

Why do we use a different method for the bound and the scattering states? The reason is that if we propagate a bound solution outwards from the first to the second classically forbidden (asymptotic) region we could encounter a numerical instability in the form of divergence of the numerical solution. Why? This is because in the classically forbidden region ($E < V(r)$) there are two solutions of the Schrödinger equation

$$u_l^{0,(+)}(\kappa r) \sim \exp[-\kappa r], \quad (5.31)$$

$$u_l^{0,(-)}(\kappa r) \sim \exp[+\kappa r]. \quad (5.32)$$

We're interested only in the physical one which behaves like $u_l^{0,(+)}(\kappa r)$. Nevertheless, any numerical inaccuracy introduced in the course of the forward propagation up to the entrance point into the second classically allowed region is equivalent to introducing an admixture (however small) of the unwanted exponentially diverging solution:

$$u_{l,\text{Numerov}}(kr) = u_l(kr) + \epsilon u_l^{0,(+)}(kr), E < V(r), \quad (5.33)$$

where $u_l(kr)$ is the exact solution. There will always be some inaccuracy in a numerical propagation. Eventually, the exponentially growing contamination completely takes over in magnitude and obscures the physically relevant solution. The same problem would occur, of course, if we propagated inwards from the asymptotic region since then in the first (i.e. closest to $r = 0$) classically forbidden region the solution would again pick up the unwanted exponentially increasing solution $\sim \exp[-\kappa r]$. The cure for this problem is precisely the method described above: propagate inwards and outwards from both asymptotic regions without entering the classically forbidden region twice. This is ensured by matching the two pieces of the wavefunction inside the classically allowed region, e.g. at the well-defined point r_M.

It is clear now why we didn't have to employ this approach for the scattering states (i.e. $k > 0$): either there is no classically forbidden region (usually for $l = 0$) or there is typically only one such region close to the origin (in case of $l > 0$), where the angular momentum barrier dominates. Perhaps there can be one or more classically forbidden sections for larger r if there are "tunneling" regions in the effective potential. However, these regions tend to be fairly short and the barrier small so typically the pure outwards propagation works well.

Nevertheless we note that we could obtain the phase shifts using the same approach as for the bound states: propagate for the given energy (momentum), inwards from the potential-free region Eq (5.4) starting with some guess for $\delta_l(k)$ and an arbitrary

normalization N and propagate outwards from $r = 0$ as described above. The correct phase shift for momentum k is the one for which the two pieces of the wavefunction join smoothly at $r = r_M$.